

Time Fractional Schrödinger Equation; Fox's H-functions and the Effective Potential

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After introducing the formalism of the general space and time fractional Schrödinger equation, we concentrate on the time fractional Schrödinger equation and present new results via the elegant language of Fox's H-functions. We show that the general time dependent part of the wave function for the separable solutions of the time fractional Schrödinger equation is the Mittag-Leffler function with an imaginary argument by two different methods. After separating the Mittag-Leffler function into its real and imaginary parts, in contrast to existing works, we show that the total probability is ≤ 1 and decays with time. Introducing the effective potential approach, we also write the Mittag-Leffler function with an imaginary argument as the product of its purely decaying and purely oscillating parts. In the light of these, we reconsider the simple box problem.

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I. INTRODUCTION

The history of fractional calculus can be traced all the way back to Leibniz. In a letter to L'Hopital (1695), Leibniz mentions that he has an expression that looks like a fractional derivative [1, 2]. Later, Euler notices that using his gamma function fractional integrals may be possible. However, a systematic development of the subject does not come until nineteenth century, where Riemann, Liouville, Grünwald and Letnikov play key roles [1-6]. On the application side, after it became clear that anomalous diffusion can be investigated in terms of the fractional diffusion equation, the situation has been changing rapidly [1-6]. The first applications to quantum mechanics started with Laskin in 2000, where he considered the path integral formulation of quantum mechanics over Lévy paths and showed that the corresponding equation of motion is the space fractional Schrödinger equation [7-17]. In

2004, Naber [18] discussed the time fractional Schrödinger equation [18-24] and obtained the time dependent part of the wave function for the separable solutions as the Mittag-Leffler function with an imaginary argument, which he wrote as a purely oscillatory term plus an integral that can not be evaluated analytically by standard techniques [18]. The main arguments and the conclusions of the paper were based on the *critical* assumption that this integral is uniformly decaying, hence could be neglected for sufficiently large times. This affected the main conclusions of the paper by giving probabilities greater than 1. Later, others have also followed this *critical* assumption [22-24].

We evaluate this integral exactly by using the elegant language of Fox's H -functions [25-27] and show that the decomposition of the Mittag-Leffler function as the sum of its purely oscillating and purely decaying parts is not possible. Since this point implies dramatic changes in the conclusions of the previous works [18, 22-24], we reconsider the problem of the time fractional Schrödinger equation.

After introducing the time and space fractional Schrödinger equation in Section II, in Section III we concentrate on the time fractional Schrödinger equation and discuss its separable solutions. We show that the time dependence is given as the Mittag-Leffler function with an imaginary argument by two different methods. After separating the Mittag-Leffler function into its real and imaginary parts, we show that the total probability is always ≤ 1 and decays with time. We also discuss the asymptotic forms of the wave function. In Section IV, we discuss the simple box problem, and in Section V, we introduce the effective potential approach. Using the effective potential, in Section VI we show that the Mittag-Leffler function with an imaginary argument can be written, not as the sum, but as the product of its purely decaying and purely oscillating parts. In Section VII, we discuss our results.

II. FRACTIONAL SCHRÖDINGER EQUATION

To write the fractional Schrödinger equation, we use the fact that the Schrödinger equation is analytic in the lower half complex t -plane, and perform a Wick rotation, $t \rightarrow -it$, on the one dimensional Schrödinger equation,

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x, t), \quad (1)$$

to write

$$-\hbar \frac{\partial \Psi}{\partial t} = -\frac{1}{2m} \left(\hbar \frac{\partial}{\partial x} \right)^2 \Psi + V(x) \Psi(x, t). \quad (2)$$

This is nothing but the Bloch equation [6]

$$\frac{\partial \Psi}{\partial t} = \check{D} \frac{\partial^2 \Psi}{\partial x^2} - \frac{1}{\hbar} V(x) \Psi(x, t), \quad \check{D} > 0, \quad (3)$$

where $\check{D} = \frac{\hbar}{2m}$ is the quantum diffusion constant and $V(x)$ is the potential. We can now write the time and space fractional version of the Bloch equation as

$${}_0^C D_t^\alpha \Psi(x, t) = \frac{1}{\hbar} \check{D}_{\alpha, \beta} \hbar^\beta R_x^\beta \Psi(x, t) - \frac{1}{\hbar} V(x) \Psi(x, t), \quad 0 < \alpha < 1, \quad 1 < \beta < 2, \quad (4)$$

where ${}_0^C D_t^\alpha$ is the Caputo derivative and R_x^β is the Riesz derivative (Appendix A). When there is no room for confusion, we also write ${}_0^C D_t^\alpha \equiv \frac{\partial^\alpha}{\partial t^\alpha}$ and $R_x^\beta \equiv \nabla^\beta \equiv \frac{\partial^\beta}{\partial x^\beta}$. We have also introduced a new quantum diffusion constant, $\check{D}_{\alpha, \beta}$, with the appropriate units. Performing an inverse Wick rotation, $t \rightarrow it$, we obtain the most general fractional version of the Schrödinger equation as

$$\frac{\partial^\alpha}{\partial t^\alpha} \Psi(x, t) = \frac{i^\alpha}{\hbar} \check{D}_{\alpha, \beta} \left(\hbar \frac{\partial}{\partial x} \right)^\beta \Psi(x, t) - \frac{i^\alpha}{\hbar} V(x) \Psi(x, t). \quad (5)$$

A. Space Fractional Schrödinger Equation

When $\alpha = 1$, Equation (5) becomes the space fractional Schrödinger equation investigated by Laskin [7]:

$$\frac{\partial}{\partial t} \Psi(x, t) = \frac{i}{\hbar} \check{D}_{1, \beta} \left(\hbar \frac{\partial}{\partial x} \right)^\beta \Psi(x, t) - \frac{i}{\hbar} V(x) \Psi(x, t), \quad (6)$$

which he wrote as

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -D_\beta [\hbar \nabla]^\beta \Psi(x, t) + V(x) \Psi(x, t). \quad (7)$$

Laskin called $[\hbar \nabla]^\beta$ the quantum Riesz derivative and D_β in the above equation is the quantum diffusion constant for the space fractional Schrödinger equation, where as $\beta \rightarrow 2$, $D_\beta \rightarrow 1/2m$.

B. Time Fractional Schrödinger Equation

For $\beta = 2$, we get

$$\frac{\partial^\alpha}{\partial t^\alpha} \Psi(x, t) = \frac{i^\alpha}{\hbar} \check{D}_{\alpha, 2} \left(\hbar \frac{\partial}{\partial x} \right)^2 \Psi(x, t) - \frac{i^\alpha}{\hbar} V(x) \Psi(x, t), \quad (8)$$

or

$$\frac{\partial^\alpha}{\partial t^\alpha} \Psi(x, t) = i^\alpha \check{D}_{\alpha,2} \hbar \frac{\partial^2}{\partial x^2} \Psi(x, t) - \frac{i^\alpha}{\hbar} V(x) \Psi(x, t). \quad (9)$$

By defining a new quantum diffusion constant, $D_\alpha = \check{D}_{\alpha,2} \hbar$, we can write the time fractional Schrödinger equation as

$$\frac{\partial^\alpha}{\partial t^\alpha} \Psi(x, t) = i^\alpha D_\alpha \frac{\partial^2}{\partial x^2} \Psi(x, t) - \frac{i^\alpha}{\hbar} V(x) \Psi(x, t), \quad 0 < \alpha < 1, \quad (10)$$

where $D_\alpha \rightarrow \hbar/2m$ as $\alpha \rightarrow 1$. Note that there is a certain amount of ambiguity in writing the time fractional version of the Schrödinger equation [18]. We will address this point again in Section VII.

III. SEPARABLE SOLUTIONS OF THE TIME FRACTIONAL SCHRÖDINGER EQUATION

We now reconsider the time fractional Schrödinger equation. Assuming a separable solution of the form $\Psi(x, t) = X(x)T(t)$, we obtain the equations to be solved for $X(x)$ and $T(t)$, respectively, as

$$D_\alpha \frac{d^2 X(x)}{dx^2} - \frac{V(x)}{\hbar} X(x) = \lambda_n X(x), \quad (11)$$

$$\frac{\partial^\alpha T(t)}{\partial t^\alpha} = i^\alpha \lambda_n T(t), \quad 0 < \alpha < 1, \quad (12)$$

where the spatial equation [Eq. (11)] has to be solved with the appropriate boundary conditions, and λ_n is the separation constant. At this point, the index n is redundant but we keep it for the cases where λ is discrete. Since in the limit as $\alpha \rightarrow 1$, $D_\alpha \rightarrow \hbar/2m$ and $\lambda_n \rightarrow -E_n/\hbar$, for physically interesting cases we will take $\lambda_n < 0$.

A. Time Dependence – Method I

Using Equation (A7) in Appendix A, we take the Laplace transform of Equation (12):

$$\mathcal{L} \left\{ \frac{\partial^\alpha T(t)}{\partial t^\alpha} \right\} = i^\alpha \lambda_n \mathcal{L} \{ T(t) \}, \quad (13)$$

to write

$$s^\alpha \tilde{T}(s) - s^{\alpha-1} T(0) = i^\alpha \lambda_n \tilde{T}(s), \quad (14)$$

where $\tilde{T}(s) = \mathcal{L}\{T(t)\}$. This gives the Laplace transform of the time dependence of the wave function as

$$\tilde{T}(s) = T(0) \frac{s^{\alpha-1}}{s^\alpha - i^\alpha \lambda_n} \quad (15)$$

$$= T(0) \frac{s^{-1}}{1 - i^\alpha \lambda_n s^{-\alpha}}. \quad (16)$$

Using geometric series, we can also write this as

$$\tilde{T}(s) = T(0) \sum_{m=0}^{\infty} (i^\alpha \lambda_n s^{-\alpha})^m s^{-1} \quad (17)$$

$$= T(0) \sum_{m=0}^{\infty} i^{\alpha m} \lambda_n^m s^{-m\alpha-1}, \quad (18)$$

which converges for $|i^\alpha \lambda_n s^{-\alpha}| < 1$. The inverse Laplace transform of this can be found easily to yield the time dependent part of the wave function as

$$T(t) = T(0) \sum_{m=0}^{\infty} \frac{i^{\alpha m} \lambda_n^m t^{\alpha m}}{\Gamma(1 + \alpha m)} \quad (19)$$

$$= T(0) \sum_{m=0}^{\infty} \frac{(i^\alpha \lambda_n t^\alpha)^m}{\Gamma(1 + \alpha m)} \quad (20)$$

$$= T(0) E_\alpha(i^\alpha \lambda_n t^\alpha), \quad (21)$$

where $E_\alpha(i^\alpha \lambda_n t^\alpha)$ is the Mittag-Leffler function with an imaginary argument.

B. Time Dependence – Method II

To find the time dependence of the wave function, an alternate path can also be taken by directly evaluating the integral [18]

$$T(t) = T(0) \left[\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{st} s^{\alpha-1} ds}{s^\alpha - i^\alpha \lambda_n} \right]. \quad (22)$$

The integrand has a pole at $s_1 = 0$ due to the numerator, and a pole at $s_2 = i\lambda_n^{1/\alpha}$ due to the denominator, hence can be rewritten as (Bayin [6] and supplements of Ch. 14, [18])

$$T(t) = T(0) \left[\frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} - \frac{\sigma \sin \alpha \pi}{\pi} \int_0^\infty \frac{e^{-xt} x^{\alpha-1} dx}{x^{2\alpha} - 2\sigma \cos \alpha \pi x^\alpha + \sigma^2} \right]. \quad (23)$$

For $\lambda_n > 0$, the above expression is valid for all $0 < \alpha < 1$. For $\lambda_n < 0$, the second pole, $s_2 = |\lambda_n|^{1/\alpha} e^{i(\pi/\alpha + \pi/2)}$, has both real and imaginary parts. Since the branch cut is

located along the negative real axis, we have to exclude the $\alpha = \frac{2}{5}, \frac{2}{9}, \frac{2}{13}, \dots$ values, that is, $\alpha = 2/(5 + 4n)$, $n = 0, 1, 2, \dots$, so that the pole lies inside the contour. We now write Equation (23) as

$$T(t) = T(0) \left[\frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} - F_\alpha(\sigma; t) \right], \quad \sigma = \lambda_n i^\alpha, \quad (24)$$

where

$$F_\alpha(\sigma; t) = \frac{\sigma \sin \alpha \pi}{\pi} \int_0^\infty \frac{e^{-xt} x^{\alpha-1} dx}{x^{2\alpha} - 2\sigma \cos \alpha \pi x^\alpha + \sigma^2}. \quad (25)$$

In previous works, the above integral was assumed to be a decaying exponential, hence neglected in subsequent calculations [18, 22-24]. This resulted in probabilities greater than 1. We now show that an exact treatment of this integral, which can not be evaluated analytically by standard techniques, proves otherwise. Using the elegant language of Fox's H- functions, details of which are presented in Appendices B and C, we evaluate the above integral exactly and show that it has an oscillatory part along with a Mittag-Leffler function as

$$F_\alpha(\sigma; t) = \pm \frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} - E_\alpha(\lambda_n i^\alpha t^\alpha). \quad (26)$$

Thus, the second method gives the time dependent part of the wave function as

$$T(t) = T(0) \left[\frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} \mp \frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} + E_\alpha(\lambda_n i^\alpha t^\alpha) \right]. \quad (27)$$

To be consistent with the robust result of Method I [Eq. (21)], we pick the minus sign, hence the time dependent part of the wave function is again obtained as

$$T(t) = E_\alpha(\lambda_n i^\alpha t^\alpha), \quad (28)$$

where without loss of any generality we have set $T(0) = 1$.

C. Probability and Asymptotic Behavior

1. Total Probability:

Since the general time dependence of the separable solutions of the time fractional Schrödinger equation is established as the Mittag-Leffler function with an imaginary ar-

gument [Eq. (28)], we can write the series

$$T(t) = E_\alpha(\lambda_n i^\alpha t^\alpha) = \sum_{\nu=0}^{\infty} \frac{(\lambda_n i^\alpha t^\alpha)^\nu}{\Gamma(1 + \alpha\nu)}, \quad |\lambda_n i^\alpha t^\alpha| < 1 \quad (29)$$

$$= \left[1 + \frac{\lambda_n i^\alpha t^\alpha}{\Gamma(1 + \alpha)} + \frac{(\lambda_n i^\alpha t^\alpha)^2}{\Gamma(1 + 2\alpha)} + \frac{(\lambda_n i^\alpha t^\alpha)^3}{\Gamma(1 + 3\alpha)} + \dots \right], \quad (30)$$

which can be separated into its real and imaginary parts as

$$E_\alpha(\lambda_n i^\alpha t^\alpha) = E_\alpha^R(t) + iE_\alpha^I(t), \quad 0 < \alpha < 1, \quad (31)$$

$$= \sum_{\nu=0}^{\infty} \frac{\lambda_n^\nu [\cos \frac{\nu\alpha\pi}{2}] t^{\alpha\nu}}{\Gamma(1 + \alpha\nu)} + i \sum_{\nu=0}^{\infty} \frac{\lambda_n^\nu [\sin \frac{\nu\alpha\pi}{2}] t^{\alpha\nu}}{\Gamma(1 + \alpha\nu)}. \quad (32)$$

When $\alpha = 1$, naturally, $E_\alpha(\lambda_n i^\alpha t^\alpha)$ becomes the Euler equation, that is,

$$T_{\alpha=1}(t) = \cos \lambda_n t + i \sin \lambda_n t \quad (33)$$

$$= e^{i\lambda_n t}. \quad (34)$$

The eigenvalues, λ_n , come from the solution of the space part of the Schrödinger equation with the appropriate boundary conditions [Eq. (11)]. Note that we can also write Equation (32) as

$$T(t) = E_\alpha \left(\lambda_n \cos^{1/\nu} \left(\frac{\nu\alpha\pi}{2} \right) t^\alpha \right) + i E_\alpha \left(\lambda_n \sin^{1/\nu} \left(\frac{\nu\alpha\pi}{2} \right) t^\alpha \right), \quad (35)$$

which in terms of H -functions becomes (Appendix B, [25])

$$T(t) = \left[H_{1,2}^{1,1} \left(-\lambda_n \cos^{1/\nu} \left(\frac{\nu\alpha\pi}{2} \right) t^\alpha \middle|_{(0,1),(0,\alpha)}^{(0,1)} \right) + i H_{1,2}^{1,1} \left(-\lambda_n \sin^{1/\nu} \left(\frac{\nu\alpha\pi}{2} \right) t^\alpha \middle|_{(0,1),(0,\alpha)}^{(0,1)} \right) \right]. \quad (36)$$

An important consequence of this result is that for the time fractional Schrödinger equation, the total probability, $\int_{-\infty}^{+\infty} |\Psi(x, t)| dx$, which is a function of time:

$$\begin{aligned} \int_{-\infty}^{+\infty} |\Psi(x, t)| dx &= |T(t)|^2 \int_{-\infty}^{+\infty} |X(x)|^2 dx \\ &= \left[|E_\alpha^R(t)|^2 + |E_\alpha^I(t)|^2 \right] \int_{-\infty}^{+\infty} |X(x)| dx \\ &= |E_\alpha^R(t)|^2 + |E_\alpha^I(t)|^2, \end{aligned} \quad (37)$$

is not conserved. The normalization constant is fixed by the total probability at $t = 0$:

$$\int_{-\infty}^{+\infty} |\Psi(x, 0)| dx = \int_{-\infty}^{+\infty} |X(x)| dx = 1. \quad (38)$$

2. Small Time Behavior:

For small times, we use the H -function representation of the Mittag-Leffler function:

$$E_\alpha(z) = H_{1,2}^{1,1} \left(-z_{(0,1),(0,\alpha)}^{(0,1)} \right), \quad (39)$$

and write the time dependence as

$$T(t) = H_{1,2}^{1,1} \left(-\lambda_n i^\alpha t^\alpha \Big|_{(0,1),(0,\alpha)}^{(0,1)} \right). \quad (40)$$

Using Equation (C3) we again obtain the series [Eq. (32)]

$$\begin{aligned} T(t) = & \left[1 + \frac{\cos(\alpha\pi/2)}{\Gamma(1+\alpha)}(\lambda_n t^\alpha) + \frac{\cos(\alpha\pi)}{\Gamma(1+2\alpha)}(\lambda_n t^\alpha)^2 + \frac{\cos(3\alpha\pi/2)}{\Gamma(1+3\alpha)}(\lambda_n t^\alpha)^3 + \dots \right] \\ & + i \left[\frac{\sin(\alpha\pi/2)}{\Gamma(1+\alpha)}(\lambda_n t^\alpha) + \frac{\sin(\alpha\pi)}{\Gamma(1+2\alpha)}(\lambda_n t^\alpha)^2 + \frac{\sin(3\alpha\pi/2)}{\Gamma(1+3\alpha)}(\lambda_n t^\alpha)^3 + \dots \right], \end{aligned} \quad (41)$$

which for small times gives the total probability as

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = |T(t)|^2 \int_{-\infty}^{+\infty} |X(x)|^2 dx \quad (42)$$

$$\simeq \left(1 + \frac{2 \cos(\alpha\pi/2)(\lambda_n t^\alpha)}{\alpha \Gamma(\alpha)} + 0(t^{2\alpha}) \right). \quad (43)$$

For $\lambda_n < 0$, this makes the total probability ≤ 1 for small times.

3. Large Time Behavior:

For large times, we use the expansion in Equation (C7) to write

$$T(t) = \sum_{v=0}^{\infty} \frac{-1}{\Gamma(1-\nu\alpha)(\lambda_n i^\alpha t^\alpha)^{1+\nu}} \quad (44)$$

$$= \left[-\frac{1}{\lambda_n i^\alpha t^\alpha} - \frac{1}{\Gamma(1-\alpha)(\lambda_n i^\alpha t^\alpha)^2} - \frac{1}{\Gamma(1-2\alpha)(\lambda_n i^\alpha t^\alpha)^3} - \dots \right]. \quad (45)$$

We can also write this in terms of its real and imaginary parts as

$$\begin{aligned} T(t) = & \left[-\frac{\cos(\alpha\pi/2)}{\lambda_n t^\alpha} - \frac{\cos(\alpha\pi)}{\Gamma(1-\alpha)(\lambda_n t^\alpha)^2} - \frac{\cos(3\alpha\pi/2)}{\Gamma(1-2\alpha)(\lambda_n t^\alpha)^3} + \dots \right] \\ & + i \left[\frac{\sin(\alpha\pi/2)}{\lambda_n t^\alpha} + \frac{\sin(\alpha\pi)}{\Gamma(1-\alpha)(\lambda_n t^\alpha)^2} + \frac{\sin(3\alpha\pi/2)}{\Gamma(1-2\alpha)(\lambda_n t^\alpha)^3} + \dots \right], \end{aligned} \quad (46)$$

In agreement with Diethelm et. al. [28], for large times, the total probability decays as

$$|T(t)|^2 \propto \frac{1}{\lambda_n^2 t^{2\alpha}}. \quad (47)$$

Since the wave function is zero on and outside the boundary, the energy does not leak out. Due to the presence of the fractional time derivative, the particle inside the infinite well is not free according to the ordinary Schrödinger equation. In Section V, we introduce the *effective potential* in terms of the ordinary Schrödinger equation, where the imaginary part of the complex effective potential describes the dissipation process. Hence, the energy is basically exchanged within the box, between the physical agent that generates the effective potential and the particle.

IV. THE BOX PROBLEM

We now consider a particle in an infinite potential well, where

$$V(x) = \begin{cases} 0 & , 0 < x < a \\ \infty & , \text{elsewhere} \end{cases}. \quad (48)$$

For the separable solutions of the time fractional Schrödinger equation [Eq. (10)], we have already determined the time dependent part [Eq. (28)] of the wave function, hence we can write $\Psi(x, t) = E_\alpha(\lambda_n i^\alpha t^\alpha) X(x)$, where the spatial part comes from the solution of Equation (11) with the appropriate boundary conditions. For the particle in a box with impenetrable walls, we solve

$$D_\alpha \frac{d^2 X(x)}{dx^2} = \lambda_n X(x), \quad \Psi(0, t) = \Psi(a, t) = 0, \quad (49)$$

which yields the eigenvalues and the eigenfunctions as

$$\lambda_n = -D_\alpha \left(\frac{n\pi}{a} \right)^2, \quad X_n(x) = C_0 \sin \left(\frac{n\pi}{a} x \right), \quad n = 1, 2, \dots, \quad D_\alpha > 0. \quad (50)$$

Since we are considering the time fractional Schrödinger equation, non locality is in terms of time, which means that the system has memory. For the separable solutions, the differential equation to be solved for the space part of the wave equation is an ordinary differential equation, hence the boundary conditions used in Eq. (49) are the natural boundary conditions

for impenetrable walls. Using the normalization condition $\int |\Psi_n(x, 0)|^2 dx = 1$, we write the complete wave function as

$$\Psi_n(x, t) = \sqrt{\frac{2}{a}} \left[\sin\left(\frac{n\pi}{a}x\right) \right] E_\alpha(\lambda_n i^\alpha t^\alpha). \quad (51)$$

The total probability is time dependent, which for small times behaves as

$$\int |\Psi_n(x, t)|^2 dx = |E_\alpha^R(t)|^2 + |E_\alpha^I(t)|^2 \quad (52)$$

$$\simeq 1 - \frac{2 \cos(\alpha\pi/2)(|\lambda_n| t^\alpha)}{\alpha\Gamma(\alpha)} + 0(t^{2\alpha}), \quad (53)$$

and for large times decays as

$$\lim_{t \rightarrow \infty} \int |\Psi_n(x, t)|^2 dx \sim \frac{1}{\lambda_n^2 t^{2\alpha}} \rightarrow 0. \quad (54)$$

This is in contrast with the previous works [18, 22-24], where for large times the total probability is constant and greater than 1:

$$\lim_{t \rightarrow \infty} \int |\Psi_n(x, t)|^2 dx = \frac{1}{\alpha^2} \geq 1. \quad (55)$$

A. The Energy Operator and the Box Problem

For the time fractional Schrödinger equation, we take the new energy operator as

$$E = -\frac{\hbar}{i^\alpha} \frac{\partial^\alpha}{\partial t^\alpha}, \quad (56)$$

where the Hamiltonian is

$$H_\alpha = -D_\alpha \hbar \frac{\partial^2}{\partial x^2} + V(x). \quad (57)$$

With this operator, the energy values are real but time dependent:

$$\begin{aligned} E &= -\frac{\hbar}{i^\alpha} \int \Psi^*(x, t) \frac{\partial^\alpha}{\partial t^\alpha} \Psi(x, t) dx \\ &= -\hbar \lambda_n |E_\alpha(\lambda_n i^\alpha t^\alpha)|^2 \int |X(x)|^2 dx \\ &= -\hbar \lambda_n |E_\alpha(\lambda_n i^\alpha t^\alpha)|^2 \end{aligned} \quad (58)$$

For the box problem, the energy eigenvalues are now obtained as

$$E_n = -\frac{\hbar}{i^\alpha} \int \Psi_n^*(x, t) \frac{\partial^\alpha}{\partial t^\alpha} \Psi_n(x, t) dx, \quad (59)$$

$$= \frac{\hbar \pi^2 n^2 D_\alpha}{a^2} \left[|E_\alpha^R(t)|^2 + |E_\alpha^I(t)|^2 \right] \quad (60)$$

which for small times are given as

$$E_n \simeq \frac{\hbar\pi^2 n^2 D_\alpha}{a^2} \left(1 - \frac{2 \cos(\alpha\pi/2)(|\lambda_n| t^\alpha)}{\alpha\Gamma(\alpha)} \right).$$

For large times ($\alpha \neq 1$), the system dissipates all of its energy as

$$\lim_{t \rightarrow \infty} E_n \sim \frac{\hbar\pi^2 n^2 D_\alpha}{a^2 \lambda_n^2 t^{2\alpha}} \rightarrow 0. \quad (61)$$

In the limit as $\alpha \rightarrow 1$, $D_\alpha \rightarrow \hbar/2m$, the energy eigenvalues approach to their usual values predicted by the Schrödinger equation:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}. \quad (62)$$

Note that the ordinary energy operator, $i\hbar \frac{\partial}{\partial t}$, yields complex eigenvalues, which only in the limit as $t \rightarrow \infty$ approach to real values that are larger than their usual values in Equation (62) by a factor of $1/\nu^2$.

V. THE EFFECTIVE POTENTIAL

To gain a better understanding of the effects of the fractional time derivative, we look for an effective potential in the (ordinary) Schrödinger equation that yields the same wave function. For simplicity we will set $V(x) = 0$ in Equation (11). We now use the following useful formula [18]:

$$\frac{dT(t)}{dt} = {}^C_0 D_t^{1-\alpha} [{}^C_0 D_t^\alpha T(t)] + \frac{[{}^C_0 D_t^\alpha T(t)]_{t=0}}{\Gamma(\alpha)t^{1-\alpha}}, \quad (63)$$

which is particularly helpful in isolating and exploring the effects of fractional time derivatives in terms of an effective potential. Using separable solutions of the time fractional Schrödinger equation [Eq. (12)], we can write

$$\frac{dT(t)}{dt} = i^\alpha \lambda_n \left[{}^C_0 D_t^{1-\alpha} T(t) + \frac{T(0)}{\Gamma(\alpha)t^{1-\alpha}} \right]. \quad (64)$$

The quantity inside the square brackets is nothing but the Riemann-Liouville derivative [Eq. (A5)], thus

$$\frac{dT(t)}{dt} = i^\alpha \lambda_n [{}_0^{R-L} D_t^{1-\alpha} T(t)]. \quad (65)$$

To define an effective potential for the separable solutions, we also write the (ordinary) Schrödinger equation as

$$i\hbar \frac{dT(t)}{dt} X(x) = -\frac{\hbar^2}{2m} \frac{d^2 X(x)}{dx^2} T(t) + V_{eff.}(t) X(x) T(t), \quad (66)$$

and substitute the wave function found from the solution of the time fractional Schrödinger equation [Eq. (65) and Eq. (11) with $V(x) = 0$]:

$$i\hbar i^\alpha \lambda_n \left[{}^{R-L}_0 D_t^{1-\alpha} T(t) \right] X(x) = -\frac{\hbar^2}{2m} \frac{\lambda_n}{D_\alpha} X(x) T(t) + V_{eff.}(t) X(x) T(t), \quad (67)$$

This yields the effective potential as

$$V_{eff.}(t) = i^{1+\alpha} \hbar \lambda_n \frac{{}^{R-L}_0 D_t^{1-\alpha} T(t)}{T(t)} + \frac{\hbar^2}{2m} \frac{\lambda_n}{D_\alpha}. \quad (68)$$

Since the time dependence is given as $T(t) = E_\alpha(\lambda_n i^\alpha t^\alpha)$, we can also write

$$V_{eff.}(t) = i^{1+\alpha} \hbar \lambda_n \frac{{}^{R-L}_0 D_t^{1-\alpha} E_\alpha(\lambda_n i^\alpha t^\alpha)}{E_\alpha(\lambda_n i^\alpha t^\alpha)} + \frac{\hbar^2}{2m} \frac{\lambda_n}{D_\alpha}. \quad (69)$$

In the limit as $\alpha \rightarrow 1$, $D_\alpha \rightarrow \frac{\hbar}{2m}$, the Mittag-Leffler function becomes the exponential function, $T(t) = e^{i\lambda_n t}$, hence the effective potential vanishes as it should. With this effective potential, the Schrödinger equation yields the same wave function as the time fractional Schrödinger equation and satisfies the same boundary conditions. In other words, the wave function found from the time fractional Schrödinger equation, satisfies the Schrödinger equation with the above effective potential.

Using the H -function [25] representation of the Mittag-Leffler function (Appendix B):

$$E_\alpha(\lambda_n i^\alpha t^\alpha) = H_{1,2}^{1,1} \left(-\lambda_n i^\alpha t^\alpha \middle|_{(0,1),(0,\alpha)}^{(0,1)} \right) \quad (70)$$

and Equation (B7) for the Riemann-Liouville derivative of the H -function, we can also write the following closed expression for the effective potential:

$$V_{eff.}(t) = \frac{(i^{1+\alpha} \hbar \lambda_n)}{t^{1-\alpha}} \frac{H_{2,3}^{1,2} \left(-\lambda_n i^\alpha t^\alpha \middle|_{(0,1),(0,\alpha),(1-\alpha,\alpha)}^{(0,\alpha),(0,1)} \right)}{H_{1,2}^{1,1} \left(-\lambda_n i^\alpha t^\alpha \middle|_{(0,1),(0,\alpha)}^{(0,1)} \right)} + \frac{\hbar^2}{2m} \frac{\lambda_n}{D_\alpha}. \quad (71)$$

Using the symmetries of the H -function [25], we can further simplify the above equation as

$$V_{eff.}(t) = \frac{(i^{1+\alpha} \hbar \lambda_n)}{t^{1-\alpha}} \frac{H_{1,2}^{1,1} \left(((-\lambda_n)^{1/\alpha} i t)^\alpha \middle|_{(0,1),(1-\alpha,\alpha)}^{(0,1)} \right)}{H_{1,2}^{1,1} \left(-\lambda_n i^\alpha t^\alpha \middle|_{(0,1),(0,\alpha)}^{(0,1)} \right)} + \frac{\hbar^2}{2m} \frac{\lambda_n}{D_\alpha}, \quad (72)$$

or as

$$V_{eff.}(t) = \frac{(i^{1+\alpha} \hbar \lambda_n)}{t^{1-\alpha}} \frac{E_{\alpha,\alpha}(\lambda_n i^\alpha t^\alpha)}{E_\alpha(\lambda_n i^\alpha t^\alpha)} + \frac{\hbar^2}{2m} \frac{\lambda_n}{D_\alpha}, \quad (73)$$

where

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta \in \mathbb{C}, \quad \text{Re}(\alpha) > 0, \quad \text{Re}(\beta) > 0, \quad z \in \mathbb{C}, \quad (74)$$

is the generalized Mittag-Leffler function, and $E_{\alpha,1}(z) = E_\alpha(z)$ [25].

A. Hamiltonian

Since the effective potential is time dependent and complex, the energies corresponding to the operator $i\hbar \frac{\partial}{\partial t}$ are also time dependent and complex, that is, the ordinary Hamiltonian operator:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{eff.}(t) \quad (75)$$

is not hermitian. However, complex potentials in quantum mechanics have found interesting applications in the study of dissipative systems [29-32].

Let us now write the effective potential for the time fractional Schrödinger equation explicitly. Using Equation (73) and the expression

$$E_{\alpha,\alpha}(\lambda_n i^\alpha t^\alpha) = \sum_{k=0}^{\infty} \frac{\lambda_n^k \cos(k\alpha\pi/2) t^{\alpha k}}{\Gamma(1+k\alpha)} + i \sum_{k=0}^{\infty} \frac{\lambda_n^k \sin(k\alpha\pi/2) t^{\alpha k}}{\Gamma(1+k\alpha)}, \quad (76)$$

we can write the effective potential in terms of its real and imaginary parts as

$$V_{eff.}(t) = V_{eff.}^R(t) + iV_{eff.}^I(t), \quad (77)$$

where

$$\begin{aligned} V_{eff.}^R(t) &= \frac{\hbar^2 \lambda_n}{2m D_\alpha} - \frac{\hbar \lambda_n \sin(\alpha\pi/2) t^{\alpha-1}}{\Gamma(\alpha)} \\ &\quad - \hbar \lambda_n^2 \sin(\alpha\pi) \left(\frac{1}{\Gamma(2\alpha)} - \frac{1}{\Gamma(1+\alpha)\Gamma(\alpha)} \right) t^{2\alpha-1} + \dots \end{aligned} \quad (78)$$

and

$$\begin{aligned} V_{eff.}^I(t) &= \frac{\hbar^2 \lambda_n}{2m D_\alpha} - \frac{\hbar \lambda_n \cos(\alpha\pi/2) t^{\alpha-1}}{\Gamma(\alpha)} \\ &\quad + \hbar \lambda_n^2 \sin(\alpha\pi) \left(\frac{1}{\Gamma(1+\alpha)\Gamma(\alpha)} + \frac{\cos(\alpha\pi)}{\Gamma(2\alpha)} - \frac{2 \cos^2(\alpha\pi/2)}{\Gamma(\alpha)\Gamma(1+\alpha)} \right) t^{2\alpha-1} + \dots \end{aligned} \quad (79)$$

The imaginary part of the complex effective potential plays an important role in describing the decay of the energy of the stationary states of the time-fractional Schrödinger equation.

VI. THE MITTAG-LEFFLER FUNCTION, $E_\alpha(\lambda_n i^\alpha t^\alpha)$, AND ITS PURELY DECAYING AND OSCILLATING PARTS

Solving the Schrödinger equation [Eq. (66)] with the above effective potential, we now obtain the following expression for the time dependent part of the separable solutions of the time fractional Schrödinger equation:

$$T(t) = \left[\exp \left(\frac{1}{\hbar} \int_0^t V_{eff.}^I(t') dt' \right) \right] \exp \left(\frac{i}{\hbar} \left[\frac{\hbar^2 \lambda_n t}{2mD_\alpha} - \int_0^t V_{eff.}^R(t') dt' \right] \right), \quad (80)$$

where λ_n is a separation constant. This is naturally equivalent to the solution found before [Eq. (28)], that is, $T(t) = E_\alpha(\lambda_n i^\alpha t^\alpha)$. Note that when $\alpha = 1$, the effective potential vanishes, hence the time dependence reduces to

$$T(t) = \exp \left(-\frac{iE_n t}{\hbar} \right), \quad E_n = \frac{\hbar^2 \lambda_n}{2mD_1}. \quad (81)$$

In other words, the time dependent part of the separable solution of the time fractional Schrödinger equation, $E_\alpha(\lambda_n i^\alpha t^\alpha)$, can be written, not as the sum, but as the product of its purely oscillating and purely exponentially decaying/growing parts. Despite the fact that the effective potential corresponding to the time fractional Schrödinger equation is complex, the advantage of the effective potential approach is that one can use the mathematical structure of the Schrödinger theory.

Finally, using the expansion

$$\begin{aligned} V_{eff.}(t) \simeq & \left(\frac{\hbar^2 \lambda_n}{2mD_\alpha} - \frac{\hbar \lambda_n \sin(\alpha\pi/2)}{\Gamma(\alpha)} t^{\alpha-1} + 0(t^{2\alpha-1}) \right) \\ & + i \left(\frac{\hbar \lambda_n \cos(\alpha\pi/2)}{\Gamma(\alpha)} t^{\alpha-1} + 0(t^{2\alpha-1}) \right), \end{aligned} \quad (82)$$

the small time behavior of $T(t)$, to lowest order, becomes

$$T(t) \simeq \left[\exp \left(\frac{\lambda_n \cos(\alpha\pi/2)}{\alpha\Gamma(\alpha)} t^\alpha \right) \right] \cdot \left[\exp \left(\frac{i}{\hbar} \left(\frac{\hbar \lambda_n \sin(\alpha\pi/2)}{\alpha\Gamma(\alpha)} t^\alpha \right) \right) \right]. \quad (83)$$

For the box problem, where $\lambda_n = -D_\alpha \left(\frac{n\pi}{a} \right)^2$, $n = 1, 2, \dots$, $D_\alpha > 0$, the total probability decays exponentially, which for small times becomes

$$|T(t)|^2 \simeq 1 - \frac{2 \cos(\alpha\pi/2)}{\alpha\Gamma(\alpha)} |\lambda_n| t^\alpha + 0(t^{2\alpha}). \quad (84)$$

This is in accordance with our previous result [Eq. (43)] obtained from $T(t) = E_\alpha(\lambda_n i^\alpha t^\alpha)$.

VII. CONCLUSIONS

The fact that anomalous diffusion can be studied by fractional calculus has attracted researchers from many different branches of science and engineering into this intriguing branch of mathematics [1-6]. Since 60's, successful examples are given in random walk, anomalous diffusion, economics and finance. Introduction of fractional calculus into a certain branch of science is usually initiated by replacing certain derivatives in the evolution or the transport equations with their fractional counterparts. A general feature of these applications is that replacing a time derivative with its fractional counterpart basically introduces memory effects into the system and makes the process non Markovian, while a replacement of a space derivative introduces global or non local effects. However, it is important to note that not all such effects can be covered by fractional generalizations of the basic equations [20, 21].

In this paper, we first established the time dependent part of the separable solutions of the time fractional Schrödinger equation as the Mittag-Leffler function with an imaginary argument by two different methods. This showed that the total probability is ≤ 1 and decays with time. We also introduced the effective potential approach, where with the effective potential, the (ordinary) Schrödinger equation yields the same wave function, with the same boundary conditions, as that the time fractional Schrödinger equation.

For the energy, the standard operator used in Schrödinger theory, $E = i\hbar \frac{\partial}{\partial t}$, yields complex values since the corresponding Hamiltonian is complex and non hermitian. On the other hand, the operator $E = -\frac{\hbar}{i^\alpha} \frac{\partial^\alpha}{\partial t^\alpha}$, which follows naturally from the time fractional Schrödinger equation, yields real but time dependent energies [Eq. (58)]. In the light of these, we also discussed the particle in a box problem, which is essentially the prototype of a device or a detector with internal degrees of freedom. With the operator $E = -\frac{\hbar}{i^\alpha} \frac{\partial^\alpha}{\partial t^\alpha}$, the energy eigenvalues are real and time dependent, and decay with the imaginary part of the complex effective potential [Eq. (79)] as

$$E_n = \frac{\hbar \pi^2 D_\alpha n^2}{a^2} \exp \left(\frac{2}{\hbar} \int_0^t V_{eff.}^I(t') dt' \right). \quad (85)$$

Since the wave function is zero on and outside the boundary, the energy is exchanged within the box between the source of the effective potential and the particle. The imaginary part of the complex potential describes the dissipative processes involved.

Complex potentials have been very useful in the study of dissipative processes in both

classical and quantum physics. Sinha et. al. [29] have extended the factorization technique of Kuru and Negro [30] to study complex potentials in classical systems that are analogues of non hermitian quantum mechanical systems. In the context of quantum device modeling, a general non hermitian Hamiltonian operator has been investigated by Ferry et. al. [31]. They have also discussed the general behavior of complex potentials with applications to ballistic quantum dots and its implications for trajectories and histories in the dots. Barraff [32] have used uniform complex potentials to model particle capture from an incident beam by quantum wells. We have pointed out that there is a certain ambiguity in writing the time fractional Schrödinger equation. For separable solutions, the time fractional Schrödinger equation that Naber [18] and Dong and Xu [22] used gives the time dependence of the wave function as $E_\alpha(\lambda_n(-i)^\alpha t^\alpha)$. However, for the total probability [Eq. (37)] and the energy [Eq. (58)], both conventions yield the same time dependence since

$$|E_\alpha(\lambda_n(-i)^\alpha t^\alpha)| = |E_\alpha(\lambda_n i^\alpha t^\alpha)|, \quad 0 < \alpha < 1. \quad (86)$$

Appendix A: Basic Definitions

Riemann-Liouville Definition of Differintegral:

The basic definition of fractional derivative and integral, that is, differintegral, is the Riemann-Liouville (R-L) definition:

For $q < 0$, the R-L fractional integral is evaluated by using the formula

$$\left[\frac{d^q f}{[d(t-a)]^q} \right] = \frac{1}{\Gamma(-q)} \int_a^t [t-t']^{-q-1} f(t') dt', \quad q < 0. \quad (A1)$$

For fractional derivatives, $q \geq 0$, the above integral is divergent, hence the R-L formula is modified as [6]

$$\left[\frac{d^q f}{[d(t-a)]^q} \right] = \frac{d^n}{dt^n} \left[\frac{1}{\Gamma(n-q)} \int_a^t [t-t']^{-(q-n)-1} f(t') dt' \right], \quad q \geq 0, \quad n > q, \quad (A2)$$

where the integer n must be chosen as the smallest integer satisfying $(q-n) < 0$.

For $0 < q < 1$ and $a = 0$, the Riemann-Liouville fractional derivative becomes

$$\left[\frac{d^q f(t)}{dt^q} \right]_{R-L} = \frac{1}{\Gamma(1-q)} \frac{d}{dx} \int_0^t \frac{f(t') d\tau}{(t-t')^q}, \quad 0 < q < 1. \quad (A3)$$

Caputo Fractional Derivative:

In 60's Caputo introduced a new definition of fractional derivative [1-6]:

$$\left[\frac{d^q f(t)}{dt^q} \right]_C = \frac{1}{\Gamma(1-q)} \int_0^t \left(\frac{df(\tau)}{d\tau} \right) \frac{d\tau}{(t-\tau)^q}, \quad 0 < q < 1, \quad (\text{A4})$$

which was used by him to model dissipation effects in linear viscosity. The two derivatives are related by

$$\left[\frac{d^q f(t)}{dt^q} \right]_C = \left[\frac{d^q f(t)}{dt^q} \right]_{R-L} - \frac{t^{-q} f(0)}{\Gamma(1-q)}, \quad 0 < q < 1. \quad (\text{A5})$$

Laplace transforms of the Riemann-Liouville and the Caputo derivative are given as (Supplements of Ch. 14 of [6])

$$\mathcal{L} \{ {}^{R-L}_0 \mathbf{D}_t^q f(t) \} = s^q \tilde{f}(s) - \sum_{k=0}^{n-1} s^k \left({}^{R-L}_0 \mathbf{D}_t^{q-k-1} f(t) \right) \Big|_{t=0}, \quad n-1 < q \leq n, \quad (\text{A6})$$

$$\mathcal{L} \{ {}^C_0 \mathbf{D}_t^q f(t) \} = s^q \tilde{f}(s) - \sum_{k=0}^{n-1} s^{q-k-1} \frac{d^k f(t)}{dt^k} \Big|_{t=0}, \quad n-1 < q \leq n, \quad (\text{A7})$$

where ${}_a \mathbf{D}_t^q f(t) \equiv \frac{d^q f}{[d(t-a)]^q}$, and wherever there is need for distinction we use the abbreviation 'R-L' or 'C'. Since the Caputo derivative allows us to impose boundary conditions in terms of ordinary derivatives, it has found widespread use.

Riesz Derivative:

In writing the space fractional diffusion equation or the space fractional Schrödinger equation, we use the Riesz derivative, which is defined with respect to its Fourier transform (Supplements of Ch. 14 of [6])

$$\mathcal{F} \{ \mathbf{R}_t^q f(t) \} = -|\omega|^q g(\omega), \quad 0 < q < 2, \quad (\text{A8})$$

as

$$\mathbf{R}_t^q f(t) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} |\omega|^q g(\omega) e^{i\omega t} d\omega, \quad (\text{A9})$$

where $g(\omega)$ is the Fourier transform of $f(t)$. Note that

$$\mathbf{R}_t^2 f(t) = \frac{d^2}{dt^2} f(t). \quad (\text{A10})$$

Appendix B: Fox's H-Function

In 1961 Fox introduced the H -function, which gives a general way of expressing a wide range of functions encountered in applied mathematics. H -function provides an elegant

and an efficient formalism to handle problems in fractional calculus. Fox's H -function is a generalization of the Meijer's G -function and is defined with respect to a Mellin-Barnes type integral [25-27]:

$$H_{p,q}^{m,n}(z) = H_{p,q}^{m,n} \left(z \middle| \begin{smallmatrix} (a_p, A_p) \\ (b_q, B_q) \end{smallmatrix} \right) = H_{p,q}^{m,n} \left(z \middle| \begin{smallmatrix} (a_1, A_1), \dots, (a_p, A_p) \\ (b_1, B_1), \dots, (b_q, B_q) \end{smallmatrix} \right) \quad (\text{B1})$$

$$= \frac{1}{2\pi i} \int_C h(s) z^{-s} ds, \quad (\text{B2})$$

where

$$h(s) = \frac{\prod_{j=1}^m \Gamma(b_j + B_j s) \prod_{j=1}^n \Gamma(1 - a_j - A_j s)}{\prod_{j=n+1}^p \Gamma(a_j + A_j s) \prod_{j=m+1}^q \Gamma(1 - b_j - B_j s)}, \quad (\text{B3})$$

m, n, p, q are positive integers satisfying $0 \leq n \leq p$, $1 \leq m \leq q$, and empty products are taken as unity. Also, A_j , $j = 1, \dots, p$, and B_j , $j = 1, \dots, q$, are real positive numbers, and a_j , $j = 1, \dots, p$, and b_j , $j = 1, \dots, q$, are in general complex numbers satisfying

$$A_j(b_h + \nu) \neq B_h(a_j - \lambda - 1) \text{ for } \nu, \lambda = 0, 1, \dots; h = 1, \dots, m, j = 1, \dots, n. \quad (\text{B4})$$

The contour C is such that the poles of $\Gamma(b_j + B_j s)$, $j = 1, \dots, m$, are separated from the poles of $\Gamma(1 - a_j - A_j s)$, $j = 1, \dots, n$, such that the poles of $\Gamma(b_j + B_j s)$ lie to the left of C , while the poles of $\Gamma(1 - a_j - A_j s)$ are to the right of C . The poles of the integrand are assumed to be simple. The H -function is analytic for every $|z| \neq 0$ when $\mu > 0$, and analytic for $0 < |z| < 1/\beta$ when $\mu = 0$, where μ and β are defined as

$$\mu = \sum_{j=1}^q B_j - \sum_{j=1}^p A_j, \quad (\text{B5})$$

$$\beta = \prod_{j=1}^p A_j^{A_j} \prod_{j=1}^q B_j^{-B_j}. \quad (\text{B6})$$

Fox's H -function is very useful in the study of stochastic processes and in solving fractional diffusion equations [33, 34]. For example, the following useful formula for the Riemann-Liouville fractional derivative of the H -function [33]:

$${}_0^{R-L} \mathbf{D}_z^\beta \left[z^a H_{p,q}^{m,n} \left((cz)^b \middle| \begin{smallmatrix} (a_j, A_j) \\ (b_j, B_j) \end{smallmatrix} \right) \right] = z^{a-\beta} H_{p+1,q+1}^{m,n+1} \left((cz)^b \middle| \begin{smallmatrix} (-a, b), (a_j, A_j) \\ (b_j, B_j), (\beta-a, b) \end{smallmatrix} \right), \quad (\text{B7})$$

where $a, b > 0$ and $a + b \min(b_j/B_j) > -1$, $1 \leq j \leq m$, can be used to find solutions to the fractional diffusion equation by tuning the indices to appropriate values. Similarly, the Laplace transform of the H -function can be obtained by using the formula [25]

$$\mathcal{L} \left\{ x^{\rho-1} H_{p,q+1}^{m,n} \left(ax^\sigma \middle| \begin{smallmatrix} (a_p, A_p) \\ (b_q, B_q), (1-\rho, \sigma) \end{smallmatrix} \right) \right\} = s^{-\rho} H_{p,q}^{m,n} \left(as^{-\sigma} \middle| \begin{smallmatrix} (a_p, A_p) \\ (b_q, B_q) \end{smallmatrix} \right), \quad (\text{B8})$$

where the inverse transform is given as

$$\mathcal{L}^{-1} \left\{ s^{-\rho} H_{p,q}^{m,n} \left(a s^{\sigma} \middle|_{(b_q, B_q)}^{(a_p, A_p)} \right) \right\} = x^{\rho-1} H_{p+1,q}^{m,n} \left(a x^{-\sigma} \middle|_{(b_q, B_q)}^{(a_p, A_p), (\rho, \sigma)} \right), \quad (\text{B9})$$

where

$$\rho, \alpha, s \in \mathbb{C}, \quad \text{Re}(s) > 0, \quad \sigma > 0 \quad (\text{B10})$$

and

$$\text{Re}(\rho) + \sigma \max_{1 \leq i \leq n} \left[\frac{1}{A_i} + \frac{\text{Re}(a_i)}{A_i} \right] > 0, \quad |\arg a| < \frac{\pi\theta}{2}, \quad \theta = \alpha - \sigma. \quad (\text{B11})$$

Appendix C: H-Function in Computable Form

Given an H -function, we can compute, plot, and also study its asymptotic forms [25-27] by using the following series expressions:

I) If the poles of

$$\prod_{j=1}^m \Gamma(b_j + s B_j) \quad (\text{C1})$$

are simple, that is, if

$$B_h(b_j + \lambda) \neq B_j(b_h + \nu), \quad j \neq h, \quad j, h = 1, \dots, m, \quad \lambda, \nu = 0, 1, 2, \dots, \quad (\text{C2})$$

then the following expansion can be used:

$$\begin{aligned} H_{p,p}^{m,n}(z) &= \sum_{h=1}^m \sum_{\nu=0}^{\infty} \\ &= \frac{\left[\prod_{j=1}^m \Gamma(b_j - B_j(b_h + \nu)/B_h) \right] \left[\prod_{j=1}^n \Gamma(1 - a_j + A_j(b_h + \nu)/B_h) \right] (-1)^{\nu}}{\left[\prod_{j=m+1}^q \Gamma(1 - b_j + B_j(b_h + \nu)/B_h) \right] \left[\prod_{j=n+1}^p \Gamma(a_j - A_j(b_h + \nu)/B_h) \right]} \\ &\quad \times \frac{z^{(b_h + \nu)/B_h}}{\nu! B_h}, \end{aligned} \quad (\text{C3})$$

where a prime in the product means $j \neq h$. This series converges for all $z \neq 0$ if $\mu > 0$, and for $0 < |z| < 1/\beta$, if $\mu = 0$, where μ and β are defined as

$$\mu = \sum_{j=1}^q B_j - \sum_{j=1}^p A_j, \quad \beta = \prod_{j=1}^p A_j^{A_j} \prod_{j=1}^q B_j^{-B_j}. \quad (\text{C4})$$

II) If the poles of

$$\prod_{j=1}^m \Gamma(1 - a_j - sA_j) \quad (C5)$$

are simple:

$$A_h(1 - a_j + \nu) \neq A_j(1 - a_h + \lambda), \quad j \neq h, \quad j, h = 1, \dots, n, \quad \lambda, \nu = 0, 1, 2, \dots, \quad (C6)$$

then the following expansion can be used:

$$\begin{aligned} H_{p,p}^{m,n}(z) &= \sum_{h=1}^n \sum_{\nu=0}^{\infty} \\ &= \frac{\left[\prod_{j=1}^m \Gamma(1 - a_j - A_j(1 - a_h + \nu)/A_h) \right] \left[\prod_{j=1}^m \Gamma(b_j + B_j(1 - a_h + \nu)/A_h) \right]}{\left[\prod_{j=m+1}^q \Gamma(1 - b_j - B_j(1 - a_h + \nu)/A_h) \right] \left[\prod_{j=n+1}^p \Gamma(a_j + A_j(1 - a_h + \nu)/A_h) \right]}, \\ &\quad \times \frac{(-1)^\nu \left(\frac{1}{z}\right)^{(1-a_h+\nu)/A_h}}{\nu! A_h}, \end{aligned} \quad (C7)$$

where a prime in the product means $j \neq h$. This series converges for all $z \neq 0$ if $\mu < 0$, and for $|z| > 1/\beta$, if $\mu = 0$, where μ and β are defined as above.

Appendix D: The Mittag-Leffler Function

To evaluate the Mittag-Leffler function we concentrate on the integral [Eq. (25)]

$$F_\alpha(\sigma; t) = \frac{\sigma \sin \alpha \pi}{\pi} \int_0^\infty \frac{e^{-xt} x^{\alpha-1} dx}{x^{2\alpha} - 2\sigma \cos \alpha \pi x^\alpha + \sigma^2}. \quad (D1)$$

Since the Mittag-Leffler function represents behavior between a power law and an exponential, it plays a crucial role in both scientific and engineering applications. In this regard, it is imperative that we have a closed expression for this integral, which in previous works [18, 22-24] was assumed to be the purely decaying part of the Mittag-Leffler function with an imaginary argument, hence neglected in subsequent calculation with serious consequences. Since the standard methods do not allow us to evaluate this integral, we are going to use of the language of H -functions.

We start by noting that the above integral requires the evaluation of the Laplace transform

$$\mathcal{L} \left\{ \frac{x^{\alpha-1}}{x^{2\alpha} - 2\sigma \cos \alpha \pi x^\alpha + \sigma^2} \right\}. \quad (D2)$$

We first express the function

$$f(x) = \frac{1}{x^{2\alpha} - 2\sigma \cos \alpha \pi x^\alpha + \sigma^2}, \quad (D3)$$

in terms of H -functions. For this, we evaluate its Mellin transform:

$$\mathcal{M}\{f(x)\} = \widehat{f}(s) = \int_0^\infty f(x)x^{s-1}dx. \quad (\text{D4})$$

Using Equation (13.126) in Bayin [6], we evaluate the above integral to obtain the Mellin transform

$$\mathcal{M}\left\{\frac{1}{x^2 - 2\sigma \cos \alpha\pi x + \sigma^2}\right\} = -\frac{\pi(-\sigma)^{s-2} \sin \alpha(s-1)\pi}{\sin \pi s \sin \alpha\pi}, \quad (\text{D5})$$

which after using the property

$$\mathcal{M}\{f(x^\beta)\} = \frac{1}{\beta} \widehat{f}\left(\frac{s}{\beta}\right), \quad \beta > 0, \quad (\text{D6})$$

allows us to write

$$\mathcal{M}\{f(x)\} = -\frac{\pi(-\sigma)^{s/\alpha} \sin(s-\alpha)\pi}{\alpha\sigma^2 \sin \alpha\pi \sin \frac{s\pi}{\alpha}}. \quad (\text{D7})$$

We now use the relation [6]

$$\sin \pi z = \frac{\pi}{\Gamma(z)\Gamma(1-z)}, \quad (\text{D8})$$

to write

$$h(s) = \mathcal{M}\{f(x)\} = \frac{\pi}{\alpha\sigma^2 \sin \alpha\pi} \frac{(-\sigma)^{s/\alpha} \Gamma(s/\alpha) \Gamma(1-s/\alpha)}{\Gamma(\alpha-s) \Gamma(1-\alpha-s)}. \quad (\text{D9})$$

The inverse Mellin transform, which is defined as

$$g(x) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \widehat{g}(s) x^{-s} ds, \quad (\text{D10})$$

where $\widehat{g}(s)$ is the Mellin transform of $g(x)$, allows us to write

$$\begin{aligned} \frac{1}{x^{2\alpha} - 2\sigma \cos \alpha\pi x^\alpha + \sigma^2} &= \left(\frac{\pi}{\alpha\sigma^2 \sin \alpha\pi} \right) \\ &\times \left[\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{(-\sigma)^{s/\alpha} \Gamma(s/\alpha) \Gamma(1-s/\alpha)}{\Gamma(\alpha-s) \Gamma(1-\alpha-s)} x^{-s} ds \right]. \end{aligned} \quad (\text{D11})$$

Comparing with the definition of the H -function in Appendix (B):

$$H_{p,q}^{m,n} \left(z \middle| \begin{smallmatrix} (a_1, A_1), \dots, (a_p, A_p) \\ (b_1, B_1), \dots, (b_q, B_q) \end{smallmatrix} \right) = \frac{1}{2\pi i} \int_C h(s) z^{-s} ds, \quad (\text{D12})$$

we read the values of the parameters as

$$m = 1, \quad n = 1, \quad p = 2, \quad q = 2, \quad (\text{D13})$$

$$a_1 = 0, \quad A_1 = 1/\alpha, \quad a_2 = \alpha, \quad A_2 = -1, \quad (\text{D14})$$

$$b_1 = 0, \quad B_1 = 1/\alpha, \quad b_2 = \alpha, \quad B_2 = -1, \quad (\text{D15})$$

thus obtaining

$$\frac{1}{x^{2\alpha} - 2\sigma \cos \alpha\pi x^\alpha + \sigma^2} = \left(\frac{\pi}{\alpha\sigma^2 \sin \alpha\pi} \right) H_{2,2}^{1,1} \left(\frac{x}{(-\sigma)^{1/\alpha}} \middle| \begin{matrix} (0,1/\alpha), (\alpha, -1) \\ (0,1/\alpha), (\alpha, -1) \end{matrix} \right). \quad (\text{D16})$$

To evaluate $F_\alpha(\sigma; t)$, and finally the time dependence $T(t)$ of the wave function, we need the Laplace transform

$$\begin{aligned} \mathcal{L} \left\{ \frac{x^{\alpha-1}}{x^{2\alpha} - 2\sigma \cos \alpha\pi x^\alpha + \sigma^2} \right\} &= \left(\frac{\pi}{\alpha\sigma^2 \sin \alpha\pi} \right) \\ &\times \mathcal{L} \left\{ x^{\alpha-1} H_{2,2}^{1,1} \left(\frac{x}{(-\sigma)^{1/\alpha}} \middle| \begin{matrix} (0,1/\alpha), (\alpha, -1) \\ (0,1/\alpha), (\alpha, -1) \end{matrix} \right) \right\}. \end{aligned} \quad (\text{D17})$$

Using the following expression of the Laplace transform [25]:

$$\mathcal{L} \left\{ x^{\rho-1} H_{p,q}^{m,n} \left(ax^\sigma \middle| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right) \right\} = s^{-\rho} H_{p+1,q}^{m,n+1} \left(as^{-\sigma} \middle| \begin{matrix} (1-\rho, \sigma), (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right), \quad (\text{D18})$$

with the replacements

$$\rho \rightarrow \alpha, \quad a \rightarrow 1/(-\sigma)^{1/\alpha}, \quad \sigma \rightarrow 1, \quad s \rightarrow t, \quad (\text{D19})$$

$$m = 1, \quad n = 1, \quad p = 2, \quad q = 2, \quad (\text{D20})$$

$$a_1 = 0, \quad A_1 = 1/\alpha; \quad a_2 = \alpha, \quad A_2 = -1, \quad (\text{D21})$$

$$b_1 = 0, \quad B_1 = 1/\alpha; \quad b_2 = \alpha, \quad B_2 = -1, \quad (\text{D22})$$

we obtain the needed transform as

$$\begin{aligned} \mathcal{L} \left\{ \frac{x^{\alpha-1}}{x^{2\alpha} - 2\sigma \cos \alpha\pi x^\alpha + \sigma^2} \right\} &= \frac{\pi}{\alpha\sigma^2 \sin \alpha\pi} \frac{1}{t^\alpha} \\ &\times H_{2,3}^{2,1} \left((-\sigma)^{1/\alpha} t \middle| \begin{matrix} (0,1/\alpha), (1-\alpha, -1) \\ (\alpha, 1), (1, 1/\alpha), (1-\alpha, -1) \end{matrix} \right), \end{aligned} \quad (\text{D23})$$

where we have used the relation [25]

$$H_{p,q}^{m,n} \left(z \middle| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right) = H_{q,p}^{n,m} \left(\frac{1}{z} \middle| \begin{matrix} (1-b_q, B_q) \\ (1-a_p, A_p) \end{matrix} \right). \quad (\text{D24})$$

Combining these results, we finally obtain the desired integral:

$$F_\alpha(\sigma; t) = \frac{\sigma i^\alpha \sin \alpha\pi}{\pi} \int_0^\infty \frac{e^{-xt} x^{\alpha-1} dx}{x^{2\alpha} - 2\sigma \cos \alpha\pi x^\alpha + \sigma^2}, \quad (\text{D25})$$

in closed form as

$$F_\alpha(\sigma; t) = \frac{1}{\alpha\sigma t^\alpha} H_{2,3}^{2,1} \left((-\sigma)^{1/\alpha} t \middle| \begin{matrix} (0,1/\alpha), (1-\alpha, -1) \\ (\alpha, 1), (0, 1/\alpha), (1-\alpha, -1) \end{matrix} \right). \quad (\text{D26})$$

The time dependent part of the wave function [Eq. (24)] can now be written as

$$T(t) = T(0) \left[\frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} - \frac{1}{\alpha \sigma t^\alpha} H_{2,3}^{2,1} \left((-\sigma)^{1/\alpha} t \middle| \begin{smallmatrix} (0,1/\alpha), (1-\alpha,-1) \\ (\alpha,1), (0,1/\alpha), (1-\alpha,-1) \end{smallmatrix} \right) \right]. \quad (\text{D27})$$

We now use Equation (C3) to write $F_\alpha(\sigma; t)$ in computable form as

$$F_\alpha(\sigma; t) = -\frac{1}{\alpha} \sum_{\nu=0}^{\infty} (-1)^{\nu(1+\frac{1}{\alpha})} \frac{\Gamma(-\frac{\nu}{\alpha}) \Gamma(1 + \frac{\nu}{\alpha})}{\Gamma(-\nu) \nu!} \frac{(\lambda_n i^\alpha)^{\frac{\nu}{\alpha}} t^\nu}{\nu!} - \sum_{\nu=0}^{\infty} \frac{(\lambda_n i^\alpha)^\nu t^{\nu\alpha}}{\Gamma(1 + \alpha\nu)}. \quad (\text{D28})$$

Since $\mu = 1 > 0$, the above series converges for all $|z| \neq 0$. In the first series, we concentrate on the expression

$$I = (-1)^{\nu(1+\frac{1}{\alpha})} \frac{\Gamma(-\frac{\nu}{\alpha}) \Gamma(1 + \frac{\nu}{\alpha})}{\Gamma(-\nu) \nu!}. \quad (\text{D29})$$

We extend the formula

$$\frac{\Gamma(-n)}{\Gamma(-N)} = (-1)^{N-n} \frac{N!}{n!}, \quad (\text{D30})$$

where N and n are positive integers, to non integer arguments as

$$\frac{\Gamma(-q)}{\Gamma(-Q)} = (-1)^{Q-q} \frac{\Gamma(Q+1)}{\Gamma(q+1)}, \quad (\text{D31})$$

and write

$$\frac{\Gamma(-\frac{\nu}{\alpha})}{\Gamma(-\nu)} = \mp (-1)^{\nu - \frac{\nu}{\alpha}} \frac{\Gamma(\nu+1)}{\Gamma(\frac{\nu}{\alpha}+1)}. \quad (\text{D32})$$

We have inserted the \mp sign to display the ambiguity in the gamma function for the negative integer values of its argument, where it diverges as $\mp\infty$. Thus, I is evaluated as

$$I = \mp (-1)^{\nu(1+\frac{1}{\alpha})} (-1)^{\frac{\nu}{\alpha} - \nu} \frac{\Gamma(\nu+1)}{\Gamma(\frac{\nu}{\alpha}+1)} \frac{\Gamma(1 + \frac{\nu}{\alpha})}{\nu!} \quad (\text{D33})$$

$$= \mp 1. \quad (\text{D34})$$

Substituting this into $F_\alpha(\sigma; t)$ [Eq. (D28)], we obtain

$$F_\alpha(\sigma; t) = \pm \frac{1}{\alpha} \sum_{\nu=0}^{\infty} \frac{(\lambda_n i^\alpha)^{\frac{\nu}{\alpha}} t^\nu}{\nu!} - \sum_{\nu=0}^{\infty} \frac{(\lambda_n i^\alpha)^\nu t^{\nu\alpha}}{\Gamma(1 + \alpha\nu)} \quad (\text{D35})$$

$$= \pm \frac{1}{\alpha} \sum_{\nu=0}^{\infty} \frac{(i\lambda_n^{1/\alpha} t)^\nu}{\nu!} - \sum_{\nu=0}^{\infty} \frac{(\lambda_n i^\alpha t^\alpha)^\nu}{\Gamma(1 + \alpha\nu)}, \quad (\text{D36})$$

which is nothing but

$$F_\alpha(\sigma; t) = \pm \frac{e^{i\lambda_n^{1/\alpha} t}}{\alpha} - E_\alpha(\lambda_n i^\alpha t^\alpha). \quad (\text{D37})$$

Substituting this into Equation (24), we write the time dependent part of the wave function as

$$T(t) = T(0) \left[\frac{e^{i\lambda_n^{1/\alpha}t}}{\alpha} \mp \frac{e^{i\lambda_n^{1/\alpha}t}}{\alpha} + E_\alpha(\lambda_n i^\alpha t^\alpha) \right]. \quad (\text{D38})$$

To be consistent with the robust result in Equation (21), we pick the minus sign. Thus the time dependent part of the wave function is again obtained as

$$T(t) = E_\alpha(\lambda_n i^\alpha t^\alpha), \quad (\text{D39})$$

where without loss of any generality we have set $T(0) = 1$.

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